Product Data Sheet

Product Name: BCR-ABL-IN-2
Cat. No.: GC33368

Chemical Properties

Cas. No.	897369-18-5		
SMILES	O=C([C@H]1NCC2=C(C=C(N3N=C(C(C)(C)C)C=C3NC(NC4=CC=CC(Cl)=C4Cl)=O)C=C2)C1)O		
Formula	$C_{24}H_{25}Cl_2N_5O_3$	M.Wt	502.39
Solubility	Soluble in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	BCR-ABL-IN-2		

Background

BCR-ABL-IN-2 is an inhibitor of BCR-ABL1 tyrosine kinase, with IC50s of 57 nM, 773 nm for ABL1native and ABL1T315I, respectively.

BCR-ABL-IN-2 (Compound 1) contains a urea moiety to allow a hydrogen bond with the conserved K271-E286 salt bridge of ABL1, a t-butyl moiety to bind into the hydrophobic spine at the third pocket position, and a 2,3-dichlorophenyl ring to stabilize the DFG-phenylalanine F382 in the Type II-out conformation. BCR-ABL-IN-2 exhibits an IC50 of 57 nM for ABL1native and an IC50 of 773 nM for ABL1T315I[1]. Despite ABL, BCR-ABL-IN-2 can also inhibit KDR, BRaf, p38 kinase with IC50s of 1.8 μM, 0.23 μM, 6.3 nM, 43 nM, respectively[2].

[1]. Chan WW, et al. Conformational control inhibition of the BCR-ABL1 tyrosine kinase, including the gatekeeper T315I mutant, by the switch-control inhibitor DCC-2036. Cancer Cell. 2011 Apr 12;19(4):556-68. [2]. ARYL SULFONOHYDRAZIDES. US 2008/0113967 A1.

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